3-2007

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Publication Info

Published in *Acta Crystallographica Section E*, Volume E63, Issue 3, 2007, pages m695-m697.

DOI: 10.1107/S1600536807004898
Publisher's Version: http://dx.doi.org/10.1107/S1600536807004898

Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368
Editors: **W. Clegg and D. G. Watson**

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Poly[diaqua(μ_4-3-fluorophthalato-κ^4O:O:O':O'')-cadmium(II)]

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.003 Å
R factor = 0.017
wR factor = 0.042
Data-to-parameter ratio = 12.0

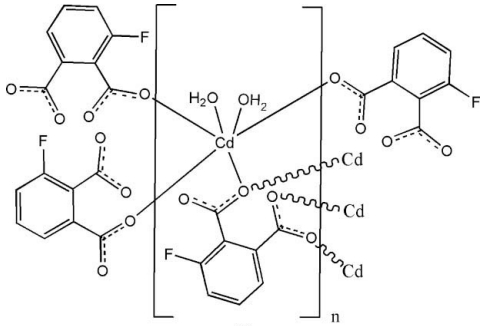
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 15 December 2006
Accepted 30 January 2007

The crystal structure of the title compound, $[Cd(C_8H_3FO_4)(H_2O)_2]_n$, consists of polymeric sheets formed by the bridging of octahedrally coordinated Cd^{II} by carboxylate O atoms of the 3-fluorophthalate (3-fpt^{2-}) ligand. The layers exhibit hydrogen bonding between each of two coordinated water molecules and two O atoms of the ligand. Adjacent sheets are connected through π–π interactions.

Comment

Polycarboxylates represent a versatile class of ligands for the construction of metal-organic coordination polymers (Ye *et al.*, 2005). Their versatility stems from the variety of bridging modes of the carboxylate group (Mehrotra & Bohra, 1983). Many of these solids exhibit properties such as gas absorption, catalytic activity, and luminescence (Rowsell *et al.*, 2004; Wasuke *et al.*, 2005; Kim *et al.*, 2004). With this in mind, the title compound, (I), was prepared as a part of our ongoing efforts to construct new coordination polymers employing polycarboxylate ligands.



(I)

The asymmetric unit consists of one Cd^{II} ion, a 3-fluorophthalate (3-fpt^{2-}) dianion, and two coordinated water molecules. The Cd^{II} ion exhibits an all-oxygen coordination in a distorted octahedral environment (Fig. 1). The axial sites are defined by a water O atom and a 3-fpt^{2-} O atom, while the equatorial sites are defined by a water O atom and three carboxylate O atoms from three equivalent 3-fpt^{2-} ligands.

The Cd—O bond distances are normal (Table 1), with an average value of 2.3031 (18) Å. All other distances and angles are comparable with those in a similar Cd^{II}–phthalate coordination polymer (Vaz *et al.*, 1996).

In (I) there are O—H···O hydrogen bonds involving three H atoms of the two water molecules and two O acceptor atoms of the 3-fpt^{2-} ligand (Table 2). The remaining water H atom along with the other two 3-fpt^{2-} O atoms are not involved in hydrogen bonding.

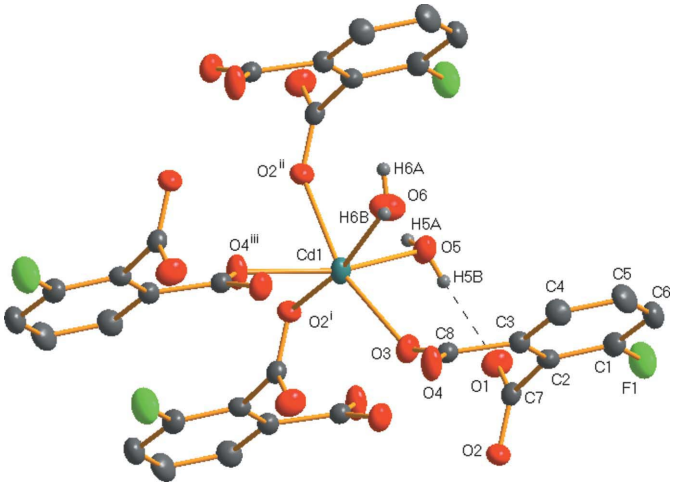


Figure 1
The coordination environment of the Cd^{II} atom in (I), showing the atom-labeling scheme. Displacement ellipsoids for non-H atoms are drawn at the 50% probability level. Hydrogen bonds are represented by dashed lines. [Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $x-1, y, z$; (iii) $-x+1, -y+2, -z+1$.]

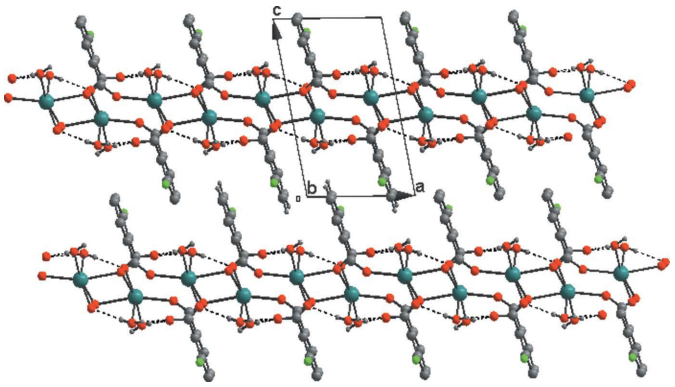


Figure 2
View of the crystal packing in (I). All H atoms, except for those of water, have been omitted for clarity. Hydrogen bonds are represented by dashed lines.

As is typical for metal phthalate-type complexes, the two carboxylate groups in (I) are not coplanar with the aromatic ring (Vaz *et al.*, 1996). One of the carboxylate groups makes a dihedral angle of 72.7 (1)°, while the other is twisted at an angle of 31.5 (1)°.

The 3-fpt^{2-} ligand acts in a μ_4-bridging fashion that links four symmetrically related Cd^{II} centers. The result is the formation of a 14-membered ring, an eight-membered ring, and a four-membered ring with Cd···Cd distances of 5.6292 (4), 4.2213 (3), and 3.7270 (3) Å, respectively. The center of each ring corresponds to a crystallographic inversion center.

The aforementioned bridging of Cd^{II} centers in (I) results in the formation of thick polymeric sheets that are stacked along the *c* axis, with the benzene rings of the 3-fpt^{2-} ligands projecting outward from each side (Fig. 2). Adjacent sheets are connected through π–π interactions involving the protruding aromatic rings of 3-fpt^{2-} from successive layers, with a centroid–centroid distance of 3.67 (2) Å between rings.

Experimental

All chemicals and solvents were purchased from commercial sources and used without further purification. 3-Fluorophthalic acid (3 mmol) was added to 100 ml of water and subsequently brought to pH 6.5 by the addition of 3 *M* NaOH with constant stirring. To this solution was added 10 ml of a 0.10 *M* solution of $Cd(NO_3)_3{\cdot}4H_2O$. Single crystals of (I) were obtained in two weeks after slow evaporation of this solution.

Crystal data

$[Cd(C_8H_3FO_4)(H_2O)_2]$
M_r = 330.54
Triclinic, $P\overline{1}$
a = 6.9460 (5) Å
b = 7.2330 (5) Å
c = 10.8199 (8) Å
α = 103.217 (1)°
β = 93.351 (1)°
γ = 115.066 (1)°
V = 471.86 (6) Å^3
Z = 2
D_x = 2.326 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 2.34 mm^{-1}
T = 294 (2) K
Irregular cleavage fragment, colorless
0.36 × 0.22 × 0.16 mm

Data collection

Bruker SMART APEX CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2003)
T_{min} = 0.882, T_{max} = 1.000
(expected range = 0.607–0.688)
4370 measured reflections
1927 independent reflections
1893 reflections with $I > 2\sigma(I)$
R_{int} = 0.012
θ_{max} = 26.4°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.017
$wR(F^2)$ = 0.042
S = 1.11
1927 reflections
161 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0169P)^2 + 0.4118P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.51 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—O2^{i}	2.3226 (15)	Cd1—O4^{iii}	2.2312 (16)
Cd1—O2^{ii}	2.3951 (15)	Cd1—O5	2.2866 (17)
Cd1—O3	2.2518 (16)	Cd1—O6	2.3308 (19)
O2^{i}—Cd1—O2^{ii}	75.64 (6)	O4^{iii}—Cd1—O3	115.46 (6)
O2^{i}—Cd1—O6	167.55 (6)	O4^{iii}—Cd1—O5	157.03 (6)
O3—Cd1—O2^{i}	109.30 (6)	O4^{iii}—Cd1—O6	98.11 (7)
O3—Cd1—O2^{ii}	161.87 (6)	O5—Cd1—O2^{i}	82.75 (6)
O3—Cd1—O5	85.61 (6)	O5—Cd1—O2^{ii}	77.62 (6)
O3—Cd1—O6	82.16 (7)	O5—Cd1—O6	93.58 (7)
O4^{iii}—Cd1—O2^{i}	81.61 (6)	O6—Cd1—O2^{ii}	91.96 (6)
O4^{iii}—Cd1—O2^{ii}	82.27 (6)		

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $x-1, y, z$; (iii) $-x+1, -y+2, -z+1$.

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H5*A*···O4^{iv}	0.765 (18)	2.076 (19)	2.840 (2)	175 (3)
O5—H5*B*···O1	0.758 (19)	1.994 (19)	2.749 (2)	175 (4)
O6—H6*B*···O1^{v}	0.764 (19)	2.040 (19)	2.804 (2)	179 (5)

Symmetry codes: (iv) $x-1, y-1, z$; (v) $x, y+1, z$.

H atoms bonded to C atoms were placed in geometrically idealized positions and included as riding atoms [C—H = 0.95 Å and U_{iso}(H) = 1.2U_{eq}(C)]. The water H atoms were located in difference maps and refined with the six O—H distances restrained to be equal with an effective s.u. of 0.015 Å.

Data collection: *SMART-NT* (Bruker, 2003); cell refinement: *SAINT-Plus*-NT (Bruker, 2003); data reduction: *SAINT-Plus*-NT; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* and *DIAMOND* (Brandenburg, 2005); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2000).

Financial support from the National Science Foundation (awards CHE-0314164 and CHE-0315152) is gratefully acknowledged.

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